

Equilibration of an isolated quantum system and thermalization of its subsystem

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An isolated quantum chaotic system in a pure state in general can equilibrate and serve as a heat bath. We show that once the equilibrium is reached, any of its subsystems that is much smaller than the isolated system is thermalized so that the subsystem is governed by the Gibbs distribution. Within this theoretical framework, the celebrated superposition principle of quantum mechanics should lead to a prediction of a thermalized subsystem with multiple temperatures if the isolated system is in a superposition state of energy eigenstates of multiple distinct energy scales. This multiple temperature state is at equilibrium, completely different from a non-equilibrium state that has multiple temperatures at different parts. Possible experimental schemes to verify this prediction are discussed.

Standard textbook always starts its discussion of quantum statistical mechanics with the microcanonical ensemble where every energy eigenstate in a narrow energy range is equally possible. Mathematically, this ensemble is described by the density matrix $\rho_{\text{mc}} = \sum_n |a_n|^2 |E_n\rangle\langle E_n|$, where E_n lies in a narrow energy range $[E, E + \Delta E]$ and $|a_n|$'s are equal to each other. Microcanonical ensemble usually refers to an isolated system and should be described by a wave function. To derive the density matrix ρ_{mc} from a wave function, two postulates—equal *a priori* probability and random phases—have to be introduced. In standard textbooks, these two postulates are either explicitly stated [1] or implicitly assumed [2]. One way to understand these two postulates is to imagine that the microcanonical ensemble is not truly isolated but weakly interacting with an outside system [1]. This seems reasonable as a system that we study always interacts with an external world. However, one is always allowed to expand the system to include more systems and eventually have a truly isolated system. As a result, it is legitimate to ask whether we can derive the main results of quantum statistical mechanics starting with a truly isolated system [3]. An equivalent question is whether we can derive thermodynamics from the dynamic evolution of a wave function [4].

There have been increased efforts to address the issue of equilibration of an isolated quantum system [4–30], partly due to that an isolated quantum system can now be achieved and sustained experimentally for a reasonable long time in a highly excited state with ultra-cold atoms [31]. Much progress has been achieved through these efforts. For example, Rigol *et al.* demonstrated numerically that the momentum of an interacting boson system in a highly excited eigenstate satisfies the microcanonical prediction, giving strong support to the eigenstate thermalization hypothesis (ETH) [5–10]. It was proved analytically that an isolated quantum system satisfying certain loose conditions can indeed equilibrate [11, 12, 19, 20].

In this work we focus on quantum chaotic systems [32–34] to address the issue of equilibration of an isolated sys-

tem. We show numerically with the Henon-Heiles system that a general quantum state in a chaotic system does equilibrate after a long time evolution. This result is not only consistent with an inequality for equilibration of an isolated system obtained previously [11, 12], but also provides an intuitive picture on how this equilibration takes place. We then prove analytically that a subsystem of an isolated quantum system at equilibrium is thermalized such that it is described by the Gibbs distribution. Here we distinguish between equilibration and thermalization: a system equilibrates if its overall features no longer change with time; a system is thermalized if its state is described by the Gibbs distribution. An equilibrated system is not necessarily thermalized while a thermalized system must be at equilibrium.

A natural and surprising outcome of this theoretical framework is that a subsystem can thermalize with multiple distinct temperatures. This can happen when the isolated system is in a superposition of energy eigenstates that concentrate around different energy scales. Although to the best of our knowledge it has never been observed in nature and in experiment, a thermalized system with multiple temperatures appears unavoidable as there is no *a priori* reason that an isolated large quantum system must be in a state which is composed only of energy eigenstates from a narrow energy range. We emphasize that this multiple-temperature state is at equilibrium so that it is completely different from a state that is out of equilibrium and has different temperatures at different parts of the system or for its different degrees of freedom. Possible experimental schemes to confirm our predication are discussed.

Equilibration of an isolated quantum chaotic system.—An important result has been achieved for the equilibration of an isolated quantum system. By generalizing Reimann's result [19], Short *et al.* [11, 12] proved an inequality regarding the fluctuation of an observable A in the course of time evolution

$$\sigma_A^2 \equiv \langle |\text{tr}\{A |\psi(t)\rangle\langle\psi(t)|\} - \text{tr}(A\rho_\infty)|^2 \rangle_t \leq \frac{\|A\|^2}{d_{\text{eff}}}, \quad (1)$$

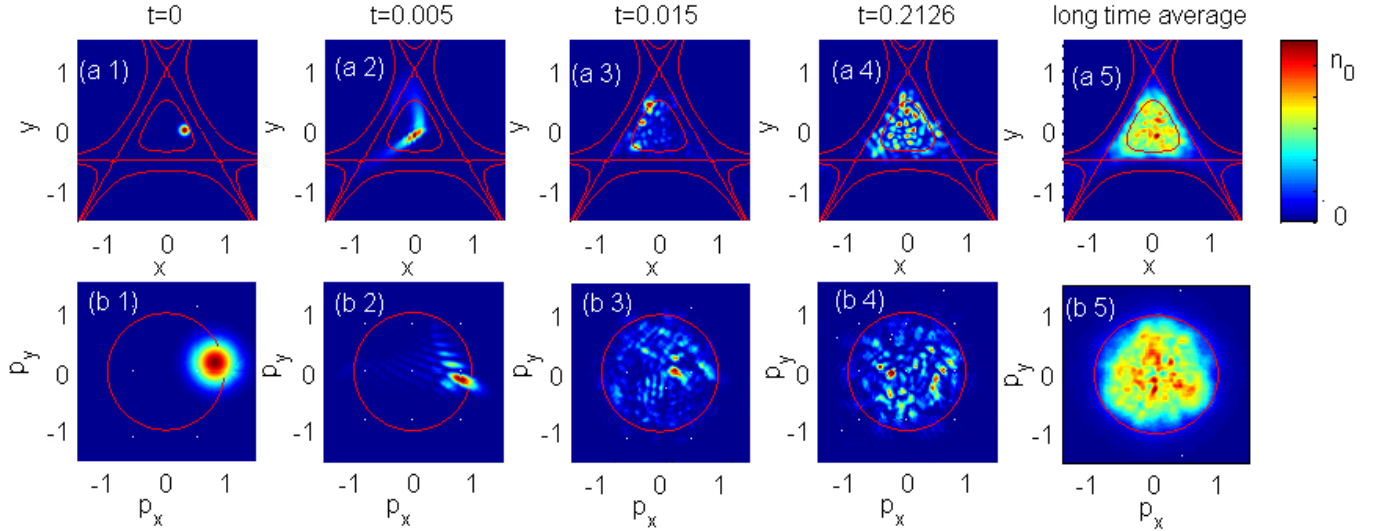


FIG. 1: Time evolution of a wave-packet and the long-time average in the Henon-Heiles system. The first row is the density in the real space and the second row is the density in the momentum space. The long-time averages of these densities are shown at the rightmost panels. The average is taken over 1200 states equally separated in the time interval of $[0.2012, 0.2255]$. The unit for the real space is r_c and the unit for the momentum space is p_0 . The red lines in the first row are energy contours of the Henon-Heiles potential at $V(x, y)/V_c = 1/2, 1, 2$. The red lines in the second row are the maximal classically allowed momentum for the initial energy of the Gaussian wave packet. The color bars are given on the right side.

where $\rho(t) = |\psi(t)\rangle \langle \psi(t)|$ with $|\psi(t)\rangle = \sum_k c_k |E_k\rangle$ being the wave function of the isolated system and $\rho_\infty = \sum_k |c_k|^2 |E_k\rangle \langle E_k|$. The subscript t in $\langle \rangle_t$ represents an averaging over a time period much longer than the characteristic time scale of the system. $\|A\|^2$ is the maximal value of A regarding all the states in the Hilbert space. The effective dimension $d_{\text{eff}} = \frac{1}{\sum_k (\text{tr}|E_k\rangle \langle E_k| \rho(t))^2}$ indicates how widely the state $|\Psi\rangle$ is spread over the energy eigenstates. For the microcanonical ensemble density matrix ρ_{mc} , one can easily check that $d_{\text{eff}} = N$ with N being the number of energy eigenstates occupied. This inequality holds for a large class of quantum systems, including quantum chaotic systems.

If a quantum system is in a state of high energy, then d_{eff} should be large since the density of states usually increases tremendously with energy. This means that the right hand side of Eq.(1) is small. For this case, this inequality tells us two things: (i) An isolated quantum chaotic system in a high-energy state will eventually equilibrate so that a bounded observable will fluctuate in small amplitude around its averaged value for almost all times. By almost all times, we mean that the fluctuation does get very large occasionally. This is similar to the familiar fact in classical statistical mechanics: even when the equilibrium is reached, large fluctuations can still occur rarely. (ii) Although the isolated quantum chaotic system is always described by a wave function, the expectation value of an observable A at almost any moment can be computed with density matrix ρ_∞ , that is, $\text{tr}(|\psi\rangle \langle \psi| A) \approx \text{tr}(\rho_\infty A)$. Note that density matrix ρ_∞ is different from the microcanonical density matrix

ρ_{cm} as $|c_k|^2$'s are determined by the initial condition and they are not necessarily equal to each other.

The inequality in Eq.(1) dictates that an isolated quantum chaotic system in high energy state can equilibrate; however, it does not show how this equilibrium is reached in a dynamical process. We now proceed to illustrate numerically this dynamical equilibration process with the Henon-Heiles system, a well-known chaotic system [35]. The Hamiltonian of the system is $H = p^2/2m + \frac{A}{2}(x^2 + y^2) + \lambda(x^2y - \frac{y^3}{3})$. The Henon-Heiles system has three saddle points located at a distance $r_c \equiv \frac{A}{\lambda}$ from the origin. These three points are the corners of the energy triangular contour with potential $V_c \equiv \frac{A^3}{6\lambda^2}$ as shown in Fig.1(a1-a5). The momentum corresponding to the saddle point energy is $p_0 \equiv \sqrt{2mV_c}$ as indicated by the circle in Fig.1(b1-b5). In our numerical simulation we set $m = \frac{1}{2}$, $\hbar = 1$, and $A/\lambda = 1/3$.

The initial condition is a highly localized Gaussian wave packet as shown in Fig.1 (a1,b1) so that the system energy is high. This wave packet is centered at $\vec{r}_i = (0.3, 0)r_c$ and $\vec{p}_i = (\cos 10^\circ, \sin 10^\circ)\sqrt{7/10}p_0$ in the real and momentum spaces, respectively. A classical particle with \vec{r}_i and \vec{p}_i has energy $0.9691V_c$. The motion of this classical particle is fully chaotic but confined in the triangular region and the circled region in the real and momentum space, respectively.

We numerically solve the time dependent Schrödinger equation and the dynamical evolution of the wave packet is illustrated in Fig.1(a1-a4,b1-b4). As the wave packet evolves, it begins to spread out and distort in shape. Eventually, it reaches an equilibrium state, where the

wave packet spreads out all over the triangular region in the real space and the circled region in the momentum space. This overall feature will no longer change even though the details of the wave packet still change in the following dynamical evolution. This is similar to the equilibrium in classical systems, where the microscopic state still changes while the overall macroscopic quantities such as pressure and temperature do not change. This kind of dynamical equilibration process has been demonstrated for chaotic billiard systems [21, 36].

For comparison, we have calculated $n_\infty(\vec{r}) = \langle \vec{r} | \rho_\infty | \vec{r} \rangle$ and $n_\infty(\vec{p}) = \langle \vec{p} | \rho_\infty | \vec{p} \rangle$ by long-time averaging, i.e. the equilibrium state obtained by Short and Reimann [11, 12, 19]. The results are shown in Fig.1(a5,b5). It is clear that $n_\infty(\vec{r})$ and $n_\infty(\vec{p})$ are very similar to the wave packet at $t = 0.2126$ with the same overall feature that the wave function spread all over both the triangular spatial region and the circled momentum region. The difference is that the wave packet at $t = 0.2126$ has larger fluctuations, whose distribution obeys an exponential law [21] while the fluctuations in both $n_\infty(\vec{r})$ and $n_\infty(\vec{p})$ are Gaussian.

To quantitatively illustrate the dynamical relaxation process, we follow the idea of Kolmogorov and Sina [37] and define an entropy as $S_\xi = \int d\xi \frac{n(\xi,t)}{n_\infty(\xi)} \ln(\frac{n(\xi,t)}{n_\infty(\xi)})$, $\xi = \vec{r}, \vec{p}$. The time evolution of S_ξ is shown in Fig.2(a1,a2). In the figure, we see clearly the entropies quickly saturate and reach the maximum values, indicating that an equilibrium state is reached. We also notice that the relaxation times in both the real and momentum spaces are about the same.

The equilibrium state reached is consistent with the inequality for equilibration obtained by Short and Reimann [11, 12, 19]. To check the inequality numerically, one needs to compute energy eigenstates of the system. As it is difficult to compute the eigenstates for the Henon-Heiles system, we have turned to the ripple billiard system studied in Ref.[21, 38], where the inequality is verified. We will present the detailed computation elsewhere and only mention that $d_{\text{eff}} \approx 300$ for a similar Gaussian wave packet in the ripple billiard system.

We have further explored the link between the quantum dynamical relaxation discussed here and its classical counterpart. For this purpose, we compare density matrix ρ_∞ with the classical microcanonical ensemble $\rho_c \equiv \frac{1}{\Omega} \delta(H(p,r) - E)$ in both the real and momentum spaces. For better comparison, we choose the following marginal distribution: for the real space, we integrate out the y dimension to obtain the density distribution $P(x)$; for the momentum space, we integrate out the angle variable to find the momentum distribution $f(p)$. The results are shown in Fig.2(b1,b2), where we see the quantum and classical distribution are consistent, except some quantum tunneling effect indicated by the non-zero value in the classically forbidden region. This link indicates that the quantum dynamical relaxation process

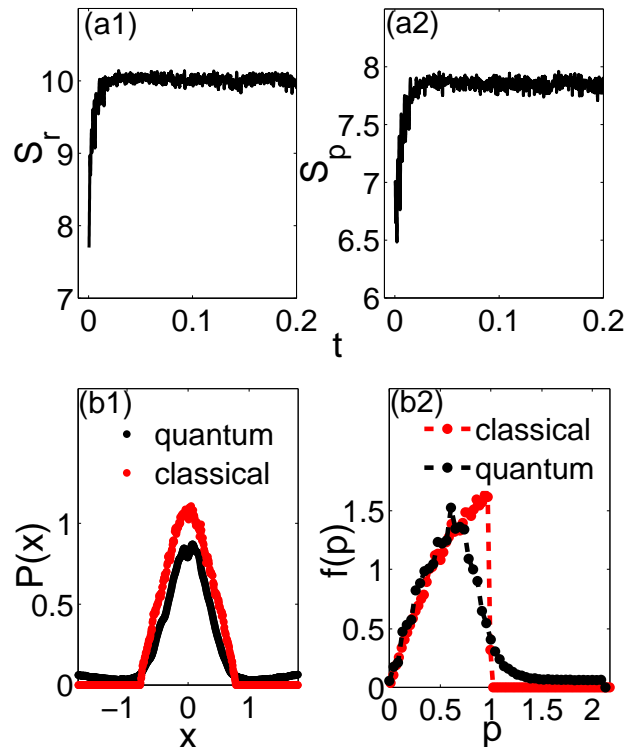


FIG. 2: (a) Time evolution of the Kolmogorov-Sina entropies S_ξ for the Henon-Heiles system for both spatial and momentum space. (b) Comparison between equilibrium quantum and classical distributions in the Henon-Heiles system. $P(x)$ is for the real space and $f(p)$ for momentum space. Unit in the real space is r_c and unit for the momentum space is p_0 .

can be understood with the help of the classical picture. Intuitively, one can think of the wave-packet as a collection of classical particles, the equilibration of a wave packet can then be likened to the relaxation process of the classical particles in the phase space. This kind of quantum-classical correspondence in dynamics has been studied before [39, 40]. However, the previous focus seems to be on the motion of the wave packet center; our focus is on the relaxation process and the final equilibrium state. Finally, we note that the quantum-classical correspondence shown in Fig.2 is not contained in the inequality Eq.(1). There is much more to be explored for the quantum dynamical relaxation in the future.

Thermalization of subsystems— We have shown that a truly isolated quantum chaotic system does equilibrate. So should any of its subsystems that are small compared to the isolated system but large enough to be considered as macroscopic objects. We shall show that due to the coupling to the rest of the system, these equilibrated subsystems are also thermalized so that they are described by the Gibbs distribution. The derivation of Gibbs distribution for a subsystem has been considered before with the assumption that the isolated system is in a pure state composed of energy eigenstates from a small

energy interval [24, 28]. We show that this assumption is not necessary and when the pure state is composed of energy eigenstates of different energy scales, the subsystem is thermalized with multiple temperatures.

We decompose the isolated quantum chaotic system into two parts, system S and thermal bath B and write the Hamiltonian as $H^{S+B} = H^S + H^B + \Delta H$, where ΔH is the weak interaction between system H^S and thermal bath H^B . Suppose that the composite system is described by a wave function $|\Phi^{S+B}\rangle = \sum c_k |E_k^{S+B}\rangle$, where $|E_k^{S+B}\rangle$'s are the energy eigenstates of the composite system. By tracing out thermal bath B , we obtain the density operator for system S , $\rho^S = \text{tr}^{(B)} |\Phi^{S+B}\rangle \langle \Phi^{S+B}|$. The system will eventually equilibrate; as an observable, ρ^S will be close to its long time average, i.e. $\rho^S \approx \langle \rho^S \rangle_t \equiv \text{tr}^{(B)} \rho_\infty^{S+B} = \text{tr}^{(B)} \sum |c_k|^2 |E_k^{S+B}\rangle \langle E_k^{S+B}|$.

We expand the eigenstate $|E_k^{S+B}\rangle$ as follows

$$|E_k^{S+B}\rangle \approx \sum' a_{ij}^k |E_i^S\rangle |E_j^B\rangle, \quad (2)$$

where $|E_i^S\rangle$ and $|E_j^B\rangle$ are energy eigenstates of system S and thermal bath B , respectively. The prime above indicates that the summation is only over eigen-energies satisfying

$$E_k^{S+B} = E_i^S + E_j^B + \Delta E_{ij}. \quad (3)$$

where ΔE_{ij} is the interaction energy that is usually very small compared to E_i^S and E_j^B when long-range interaction is negligible, e.g., gravity, in the system. Two remarks are warranted. (i) The approximation made in Eq.(2) is justified. The equality holds when there is no coupling $\Delta H = 0$. We expect it hold when the weak interaction ΔH is turned on. (ii) The weak interaction ΔH can drive the system to a state with a_{ij}^k 's randomly uniformly distributed on the sphere $\sum_{ij} |a_{ij}^k|^2 = 1$. This random distribution is similar to the idea of "typicality" [22, 23]. The connection between interaction and randomness is widely acknowledged since the details of the interaction is irrelevant to the statistical properties [41, 42]. As a result, the average value of $|a_{ij}^k|^2$ is $\frac{1}{D^{S+B}(E_k^{S+B})}$, where $D^{S+B}(E_k^{S+B})$ is the degeneracy brought by the combination of states. We emphasize that this degeneracy is different from the intrinsic degeneracy of the system and it is due to the existence of ΔE_{ij} in Eq.(3).

With the approximation made in Eq.(2), we now proceed with our derivation,

$$\begin{aligned} \rho^S &= \sum_k |c_k|^2 \sum_m \langle E_m^B | E_k^{S+B} \rangle \langle E_k^{S+B} | E_m^B \rangle \\ &= \sum_k |c_k|^2 \sum_{ii'} \left\{ \sum_m a_{im}^k a_{i'm}^{k*} \right\} |E_i^S\rangle \langle E_{i'}^S| \\ &= \sum_k |c_k|^2 \sum_i \left(\sum_m |a_{im}^k|^2 \right) |E_i^S\rangle \langle E_i^S| \end{aligned}$$

$$+ \sum_k |c_k|^2 \sum_{i \neq i'} \left(\sum_m a_{im}^k a_{i'm}^{k*} \right) |E_i^S\rangle \langle E_{i'}^S|. \quad (4)$$

The central limit theorem gives the results of the summation $\sum_m |a_{im}^k|^2 \simeq D^B(E_m^B)/D^{S+B}(E_k^{S+B})$, where $D^B(E_m^B)$ is the degeneracy of the thermal bath. There are more terms in the second summation. However, again due to the central limit theorem, the summation $\sum_m a_{im}^k a_{i'm}^{k*}$ is of the order $O\{\sqrt{D^B(E_m^B)}/D^{S+B}(E_k^{S+B})\} \simeq O\{1/\sqrt{D^{S+B}(E_k^{S+B})}\}$, where we have used that S is much smaller than B so that $D^B(E_m^B) \simeq D^{S+B}(E_k^{S+B})$. As a result, the last term in Eq.(4) has the order of magnitude at $O\{\sum_i D^S(E_i)^2 / \sqrt{D^{S+B}(E_k^{S+B})}\}$, which is practically zero for the isolated system is much larger than system S . So omitting the last term, we have from Eq.(4)

$$\rho^S = \sum_k |c_k|^2 \sum_i \frac{D^B(E_m^B)}{D^{S+B}(E_k^{S+B})} |E_i^S\rangle \langle E_i^S|. \quad (5)$$

With the standard argument for the Gibbs distribution [2], we arrive finally at

$$\rho^S = \sum_k |c_k|^2 \left\{ \sum_i \exp(-\beta_k E_i) |E_i^S\rangle \langle E_i^S| \right\}, \quad (6)$$

where $\beta_k \equiv \frac{1}{k_B T_k} \equiv \partial \ln D^{S+B}(E_k^{S+B}) / \partial E_k^{S+B}$ defines the temperature of the total system for eigenstate $|\Phi_k^{S+B}\rangle$. In this way, we have proved that a subsystem of an isolated equilibrated system is thermalized.

Thermalized state with multiple temperatures— Here we examine Eq. (6) for two typical cases: (i) The coefficients $|c_k|^2$ of the composite system have a single sharp peak distribution around energy E_p . This case is considered by others [24] in different formalisms. For this case, the density matrix ρ^S in Eq.(6) is reduced to $\rho^S = \sum_i \exp(-\beta_p E_i) |\psi_i^S\rangle \langle \psi_i^S|$. This is exactly the typical Gibbs distribution discussed in all textbook on statistical mechanics. (ii) The coefficients $|c_k|^2$ have two well-separated sharp peaks around two energies E_{p1} and E_{p2} . In other words, the composite system (or the heat bath) is in a superposition of *numerous* eigenstates centered around two very different energy scales. In this case, the thermalized system has now two temperatures, β_1 for E_{p1} and β_2 for E_{p2} , with an unconventional density matrix

$$\rho^S = \sum_i (|a_1|^2 e^{-\beta_1 E_i} + |a_2|^2 e^{-\beta_2 E_i}) |E_i^S\rangle \langle E_i^S|, \quad (7)$$

where $|a_1|^2$ and $|a_2|^2$ are the weight of the two distribution peaks. This existence of a thermalized system with more than one temperatures appears to be an unavoidable result from the superposition principle. When the heat bath is quantum, there is no *a priori* reason that

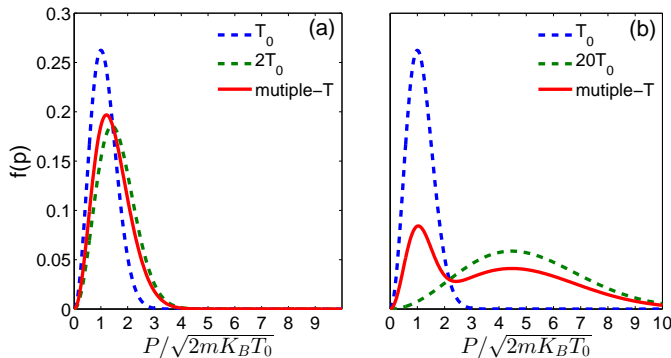


FIG. 3: Momentum distributions of a thermalized ideal gas with two temperatures. (a) The two temperatures are of the same scale; (b) the two temperatures are of different scales, and a pronounced double-peak distribution is seen. Red solid line is for the two-temperature distribution; blue dashed line for the lower temperature; green dashed line for the larger temperature.

the heat bath must be in the quantum state which is narrowly peaked at one energy. When the heat bath is in a superposition of states with well-separated energy scales, its subsystem has to thermalize with multiple temperatures.

Here are two caveats. (i) Such a state is an equilibrated state with multiple temperatures and it is completely different from the usual non-equilibrium state which has different temperatures for different parts, e.g., in the double-well experiment[43]. (ii) The isolated composite system is in a superposition of *numerous* eigenstates centered around two very different energies. This is very different from a state which is a superposition of only two different eigenstates. For the latter case, the system does not equilibrate as the right hand side of Eq.(1) is large with $d_{\text{eff}} \approx 2$; consequently, its subsystem does not thermalize.

As an example, we have computed the momentum distribution $f(P)$ of a three dimensional ideal gas that is thermalized with two temperatures. For computation, we choose $|a_1|^2 = 0.3$ and $|a_2|^2 = 0.7$ in Eq.(7) and have both temperatures much higher than the quantum degenerate temperature. Two typical results are shown in Fig.3. When the two temperatures are of the same scale, the two-temperature momentum distribution is not much different from a single temperature distribution (see Fig.3(a)); when the two temperatures are of different scale, the two-temperature state has a pronounced double-peak distribution (see Fig.3(b)), revealing the effect of two energy scales in the quantum heat bath.

For all the systems that we have encountered in nature or studied in experiment, they are in contact with classical heat bath. This may explain why such a thermalized state with multiple temperatures has never been ob-

served. However, with the advance of technology, we can now create large quantum systems such as superfluid helium and Bose-Einstein condensates (BECs), which may serve as quantum heat bath. In addition, it has been reported that the quantum and classical fluctuations can be separated out with the spin echo technique in a nuclear heat bath [44, 45]. We have also the ability to put these systems in highly excited states while keeping their coherence [31]. These technical achievements should pave the way for finally observing such an exotic thermalized state. One possible experimental scheme is to use the two-specie BECs with one specie has much larger population than the other. One may be able to drive the system to have two energy peaks with the double-well potential [43] and then observe the double-peak momentum distribution shown in Fig.3(b) for the smaller specie.

Note that Fine *et al.* have also found it not necessary to assume that a microcanonical ensemble is composed of energy states from a narrow energy range [46–48]. They replaced the standard microcanonical ensemble with “quantum microcanonical” ensemble, which is assumed to consist of all superpositions for a given energy expectation. This is fundamentally different from our approach, where no assumption for an ensemble is needed. However, physically, the quantum microcanonical” ensemble considered by Fine *et al.* may be equivalent to a special case in our theory, where the pure state of the isolated system is made of equally-weighted energy states from a wide energy range.

Summary—We have shown that a truly isolated quantum chaotic system can equilibrate and its subsystem can thermalize to the Gibbs distribution. Moreover, within such a theoretical framework we predict that the superposition principle in quantum mechanics should lead to the existence of a state that is thermalized with multiple temperatures.

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